INL/CON-22-69390-Revision-0

# TRISO Particle Anisotropies and their Impact on Fuel Performance

October 2022

Jordan Andrew Evans, Kevan D Weaver, Jackson R Harter

Idaho National Laboratory

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**Idaho National Laboratory**
**Idaho Falls, Idaho 83415**

**http://www.inl.gov**

**Prepared for the**
**U.S. Department of Energy**
**Under DOE Idaho Operations Office**
**Contract DE-AC07-05ID14517**

INL/CON-22-69390

October 19, 2022

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# TRISO Particle Anisotropies and their Impact on Fuel Performance

## The Sixth Workshop on Material Properties of TRISO Fuels

With contributions from:
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Idaho National Laboratory

# Overview

- Background
- Generalized Hooke’s Law of Elasticity
- Relating Textures to Anisotropies in TRISO Particles
- Anisotropic TRISO Fuel Performance

# BACKGROUND

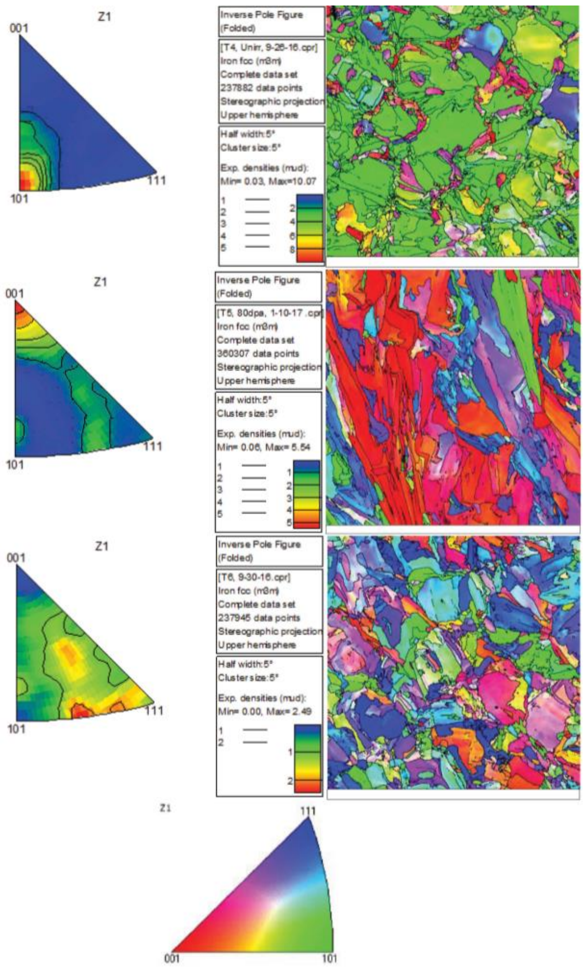
## (Texture, Anisotropy, and Hooke’s Law)

# Texture vs. Anisotropy

**Texture** relates to orientation distribution of the polycrystalline microstructure

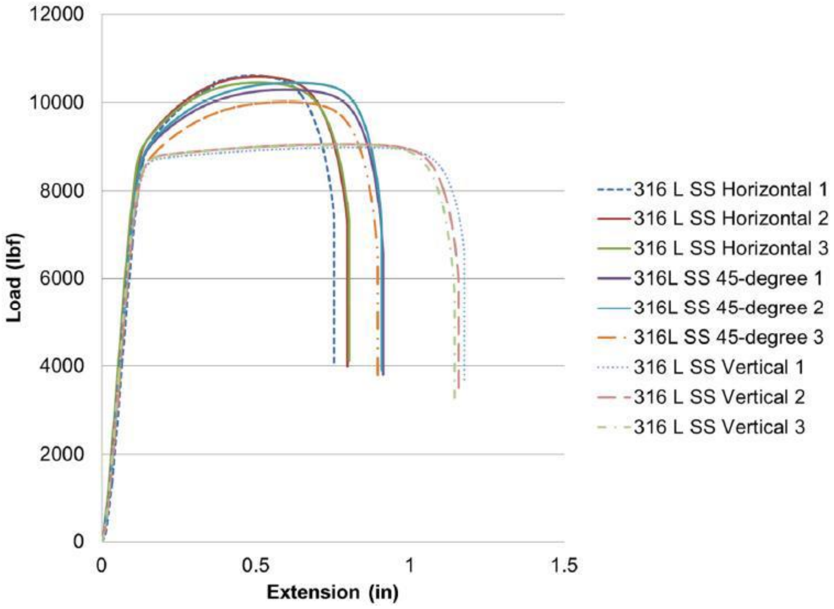
- Measured by looking at microstructure itself (ex. EBSD, XRD, 2-MGE, etc.)

[1] J.A. Evans, S.A. Anderson, E.J. Faierson, D. Perez-Nunez, S.M. McDeavitt, *Anisotropic Radiation-Induced Changes in Type 316L Stainless Steel Rods Built by Laser Additive Manufacturing*, Nucl Technol 205(4) (2019) 563-581.



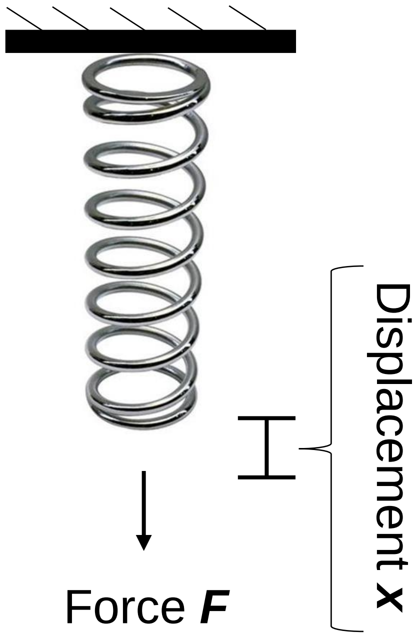
**Anisotropy** relates to the directional dependence of properties

- Measured looking at properties (ex. tensile tests in multiple directions)



**Most textured materials have anisotropic mechanical properties**

# Elasticity and Hooke’s Law (Easy Version)

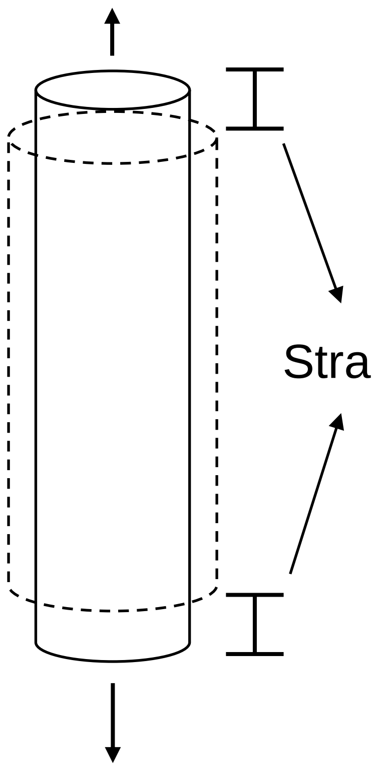


Spring

Displacement ***x***

Force ***F***

$$F = kx$$

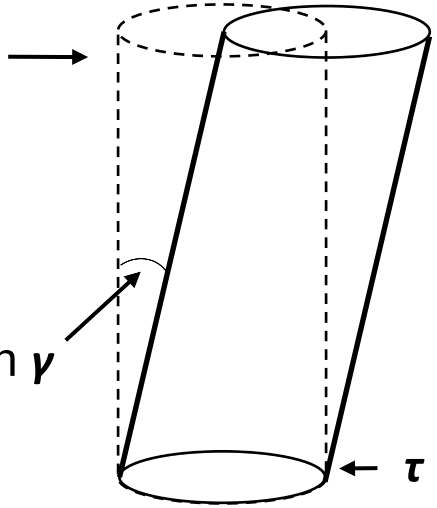


Stress ***σ***

Strain ***ε***

Stress ***σ***

$$\sigma = E\varepsilon$$



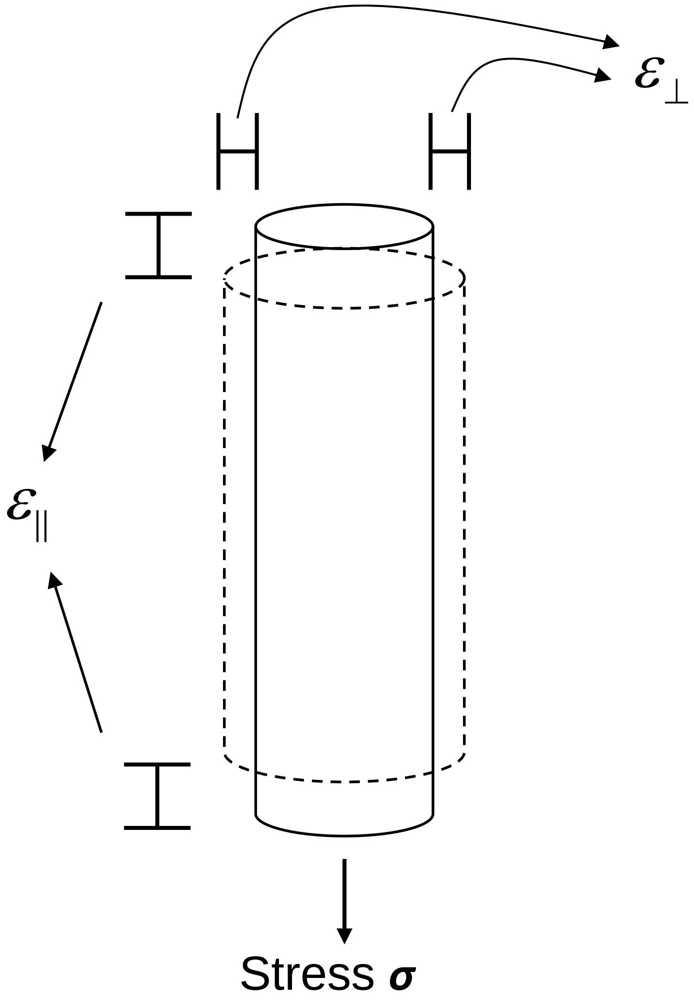
Shear Stress ***τ***

Shear Strain ***γ***

***τ***

$$\tau = G\gamma$$

# Poisson’s Ratio



$$\nu = \frac{\varepsilon_{\perp}}{\varepsilon_{\parallel}}$$

$$\sigma = E\varepsilon$$

- But if the material is textured, it *can* have anisotropic mechanical properties
- That means the “engineering constants” are not scalar and depend on orientation
  - *E*, *G*, $\nu$, etc.

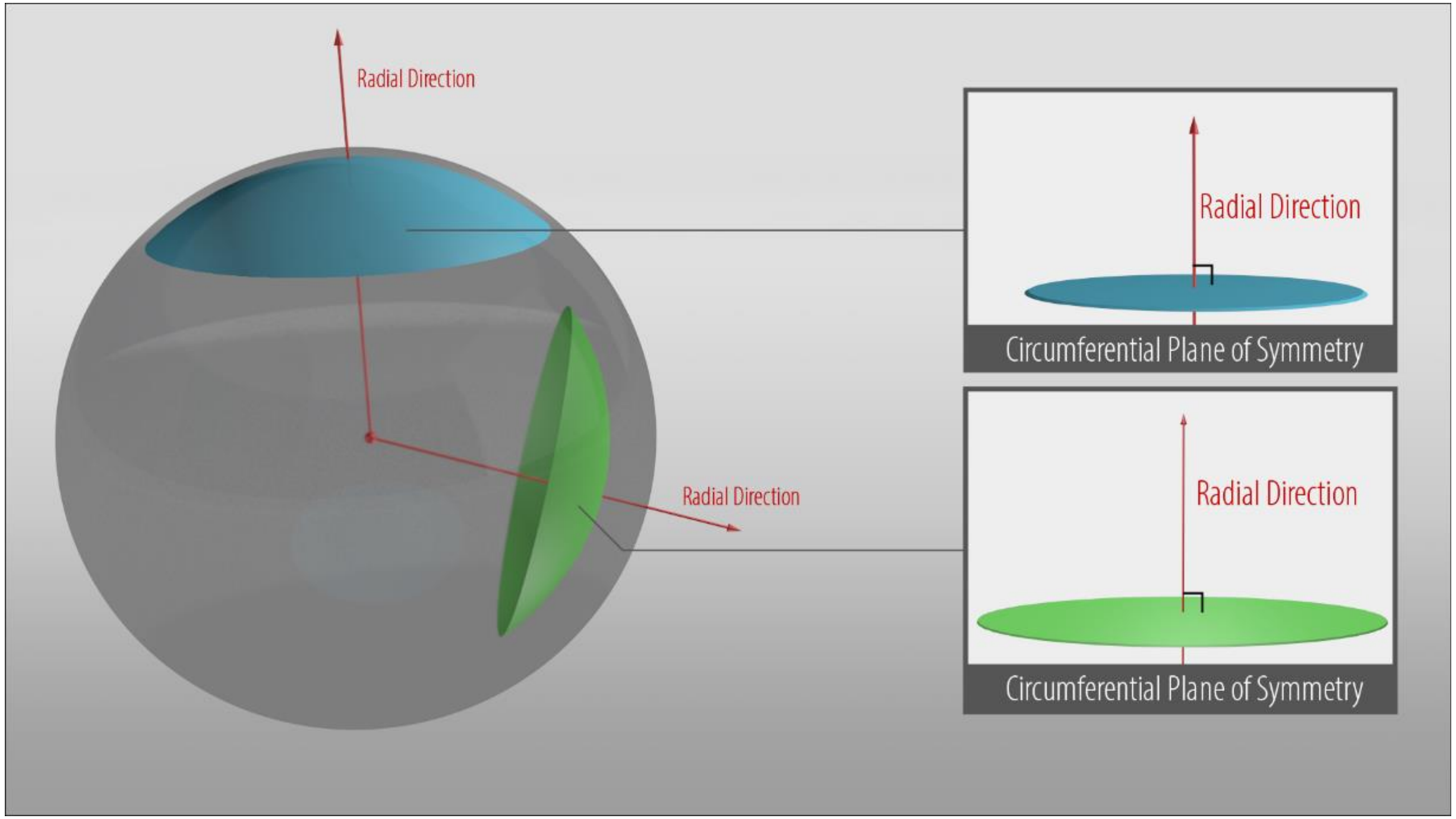
$$E = \frac{E_r + 2E_t}{3}$$

$$E_t = 25.5\left(0.384 + \rho \cdot 0.324 \times 10^{-3}\right)\left(0.481 + 0.519 \cdot BAF\right)$$
$$\left(2.985 - 0.0662 \cdot L_c\right)\left(1 + 0.23 \cdot \phi\right)\left[1 + 0.00015\left(T - 20\right)\right]$$

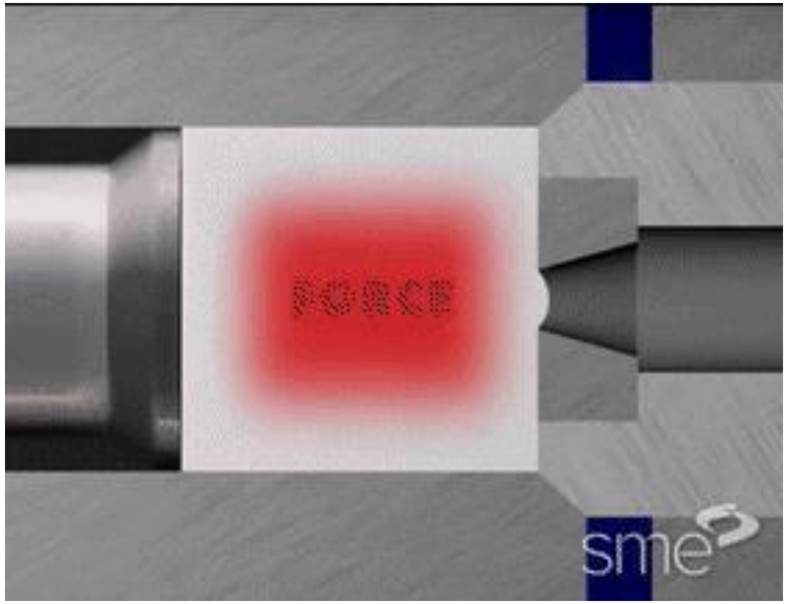
$$E_r = 25.5\left(0.384 + \rho \cdot 0.324 \times 10^{-3}\right)\left(1.463 - 0.463 \cdot BAF\right)$$
$$\left(2.985 - 0.0662 \cdot L_c\right)\left(1 + 0.23 \cdot \phi\right)\left[1 + 0.00015\left(T - 20\right)\right]$$

# Textures in TRISO Particles

TRISO particle layers tend to have (weak) textures consistent with **transversely isotropic symmetry**



(The same type of symmetry as from extrusion)



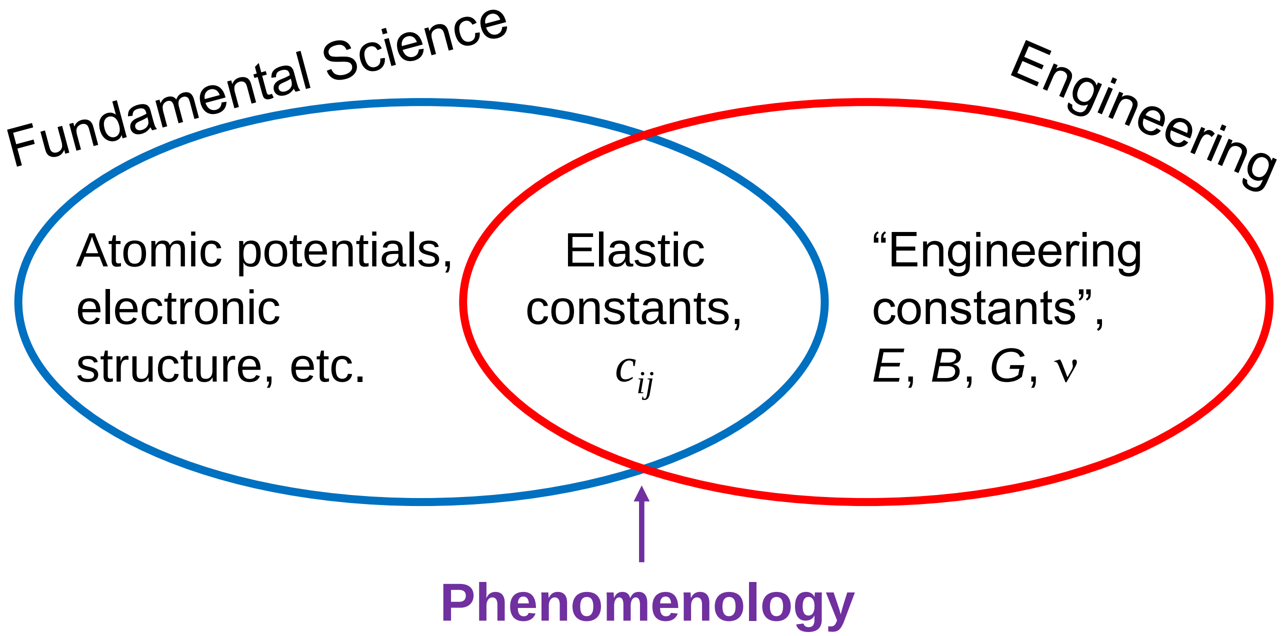
[1] J.A. Evans, R.A. Lebensohn, J.R. Harter, K.D. Weaver, *Anisotropic temperature-dependent elastic constants and thermal conductivities of TRISO particle coatings*, J Nucl Mater 565 (2022).

# GENERALIZED HOOKE'S LAW OF ELASTICITY

## (The Elastic Constants)

# Hooke’s Law and Elastic Constants

Elastic constants connect to thermodynamics, electronic structure, thermomechanical properties, etc.



Fundamental Science

Engineering

Atomic potentials, electronic structure, etc.

Elastic constants, $c_{ij}$

“Engineering constants”, *E*, *B*, *G*, $\nu$

**Phenomenology**

$$\sigma_{ij} = c_{ijkl}\varepsilon_{kl} \longrightarrow \begin{bmatrix} \sigma_{11} \\ \sigma_{22} \\ \sigma_{33} \\ \sigma_{23} \\ \sigma_{13} \\ \sigma_{12} \end{bmatrix} = \begin{bmatrix} c_{11} & c_{12} & c_{13} & c_{14} & c_{15} & c_{16} \\ & c_{22} & c_{23} & c_{24} & c_{25} & c_{26} \\ & & c_{33} & c_{34} & c_{35} & c_{36} \\ & & & c_{44} & c_{45} & c_{46} \\ & sym & & & c_{55} & c_{56} \\ & & & & & c_{66} \end{bmatrix} \begin{bmatrix} \varepsilon_{11} \\ \varepsilon_{22} \\ \varepsilon_{33} \\ 2\varepsilon_{23} \\ 2\varepsilon_{13} \\ 2\varepsilon_{12} \end{bmatrix}$$

The general form of the elastic tensor $c_{ij}$ has 21 independent constants…

# Generalized Hooke's Law

$$\boxed{\sigma_{ij} = c_{ijkl}\varepsilon_{kl}}$$

**Isotropic**: 2 independent $c_{ij}$

$$\begin{bmatrix} \sigma_{11} \\ \sigma_{22} \\ \sigma_{33} \\ \sigma_{23} \\ \sigma_{13} \\ \sigma_{12} \end{bmatrix} = \begin{bmatrix} c_{11} & c_{12} & c_{12} & 0 & 0 & 0 \\ & c_{11} & c_{12} & 0 & 0 & 0 \\ & & c_{11} & 0 & 0 & 0 \\ & & & c_{44} & 0 & 0 \\ & sym & & & c_{44} & 0 \\ & & & & & c_{44} \end{bmatrix} \begin{bmatrix} \varepsilon_{11} \\ \varepsilon_{22} \\ \varepsilon_{33} \\ 2\varepsilon_{23} \\ 2\varepsilon_{13} \\ 2\varepsilon_{12} \end{bmatrix}$$

where $c_{12} = c_{11} - 2c_{44}$

$$E_{iso} = \frac{c_{11}^2 + c_{11}c_{12} - 2c_{12}^2}{c_{11} + c_{12}}$$

$$G_{iso} = c_{44} \qquad \nu_{iso} = \frac{c_{12}}{c_{11} + c_{12}}$$

Math is a bit more complicated for transversely isotropic symmetry…

[1] J.A. Evans, B.T. Sturtevant, B. Clausen, S.C. Vogel, F.F. Balakirev, J.B. Betts, L. Capolungo, R.A. Lebensohn, B. Maiorov, *Determining elastic anisotropy of textured polycrystals using resonant ultrasound spectroscopy*, J Mater Sci 56(16) (2021) 10053-10073.

# Generalized Hooke's Law

$$\boxed{\sigma_{ij} = c_{ijkl}\varepsilon_{kl}}$$

$$E_{\parallel} = E_{rad} = \frac{c_{11}c_{33} + c_{12}c_{33} - 2c_{13}^2}{c_{11} + c_{12}}$$

$$E_{\perp} = E_{circ} = \frac{c_{11}^2 c_{33} + 2c_{13}^2 c_{12} - 2c_{13}^2 c_{11} - c_{12}^2 c_{33}}{c_{11}c_{33} - c_{13}^2}$$

$$G_{\perp\parallel} = G_{\parallel\perp} = c_{44} \qquad G_{\perp} = c_{66}$$

**Transversely Isotropic**: 5 independent $c_{ij}$

$$\begin{bmatrix} \sigma_{11} \\ \sigma_{22} \\ \sigma_{33} \\ \sigma_{23} \\ \sigma_{13} \\ \sigma_{12} \end{bmatrix} = \begin{bmatrix} c_{11} & c_{12} & c_{13} & 0 & 0 & 0 \\ & c_{11} & c_{13} & 0 & 0 & 0 \\ & & c_{33} & 0 & 0 & 0 \\ & & & c_{44} & 0 & 0 \\ & sym & & & c_{44} & 0 \\ & & & & & c_{66} \end{bmatrix} \begin{bmatrix} \varepsilon_{11} \\ \varepsilon_{22} \\ \varepsilon_{33} \\ 2\varepsilon_{23} \\ 2\varepsilon_{13} \\ 2\varepsilon_{12} \end{bmatrix}$$

where $c_{12} = c_{11} - 2c_{66}$

$$\nu_{\perp} = \frac{c_{12}c_{33} - c_{13}^2}{c_{11}c_{33} - c_{13}^2} \qquad \nu_{\parallel\perp} = \frac{c_{11}c_{13} - c_{12}c_{13}}{c_{11}^2 - c_{12}^2} \qquad \nu_{\perp\parallel} = \frac{c_{11}c_{13} - c_{12}c_{13}}{c_{11}c_{33} - c_{13}^2}$$

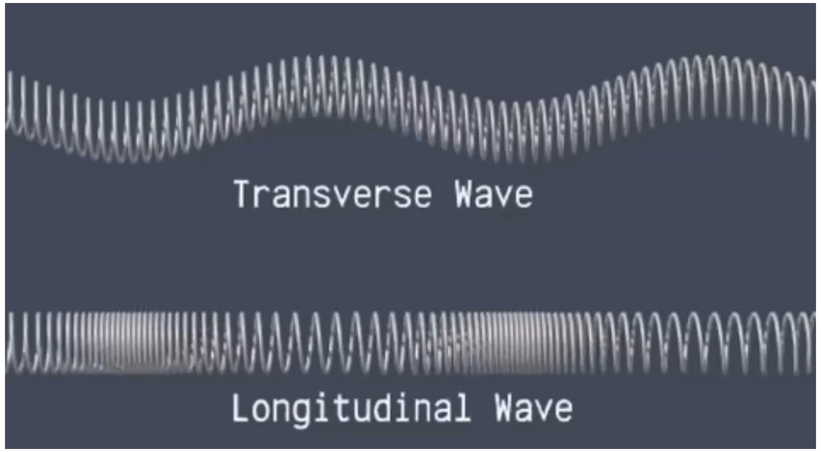
where $\nu_{ki} = \frac{\varepsilon_{kk}}{\varepsilon_{ii}}$

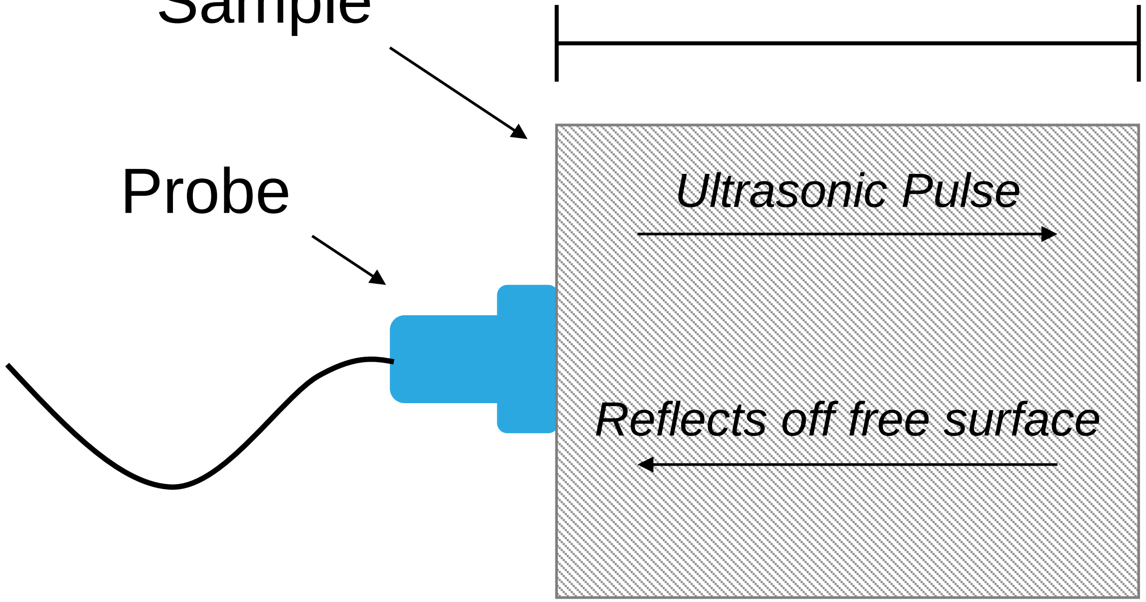
[1] J.A. Evans, B.T. Sturtevant, B. Clausen, S.C. Vogel, F.F. Balakirev, J.B. Betts, L. Capolungo, R.A. Lebensohn, B. Maiorov, *Determining elastic anisotropy of textured polycrystals using resonant ultrasound spectroscopy*, J Mater Sci 56(16) (2021) 10053-10073.

# Direct Measurement of $c_{ij}$ – Ultrasonic Pulse-Echo

$c_{44} = \rho v_T^2 \rightarrow$

$c_{11} = \rho v_L^2 \rightarrow$





Known size *x*

Sample

Probe

*Ultrasonic Pulse*

*Reflects off free surface*

Measure time-of-flight,
*v* = *x*/*t*

<u>Upsides</u> = Can be done in micro-scale samples vs. temperature
<u>Downside</u> = Must be done in multiple orientations

# RELATING TEXTURE TO ANISOTROPY IN TRISO COATINGS

# Texture to Anisotropy: The Elastic Self-Consistent (ELSC) Model

- Polycrystalline material's texture is mathematically described by a set of *crystallographic orientations* with *weights*
  - *Orientations* represent (single crystal) grains surrounded by different neighbors
  - *Weights* represent volume fractions of the grain orientations
- The surrounding medium represents the average environment surrounding the grains, and whose elastic properties need to be determined to solve the problem (Eshelby's inclusion problem)
- ELSC performs weighted averages of single crystal properties to obtain the corresponding polycrystal's bulk properties

$$\sigma_{ij} = c_{ijkl}\varepsilon_{kl}$$

$$c_{ijkl} = \left\langle c^g_{ijpq} A^g_{pqkl} \right\rangle$$

$$\tilde{c}_{ijkl} = c_{ijmn}\left(I - S\right)_{mnpq} S^{-1}_{pqkl}$$

$$A^g_{ijkl} = \left(c^g + \tilde{c}\right)^{-1}_{ijpq}\left(c + \tilde{c}\right)_{pqkl}$$

$$\varepsilon^g_{ij} = A^g_{ijkl}\,\varepsilon_{kl}$$

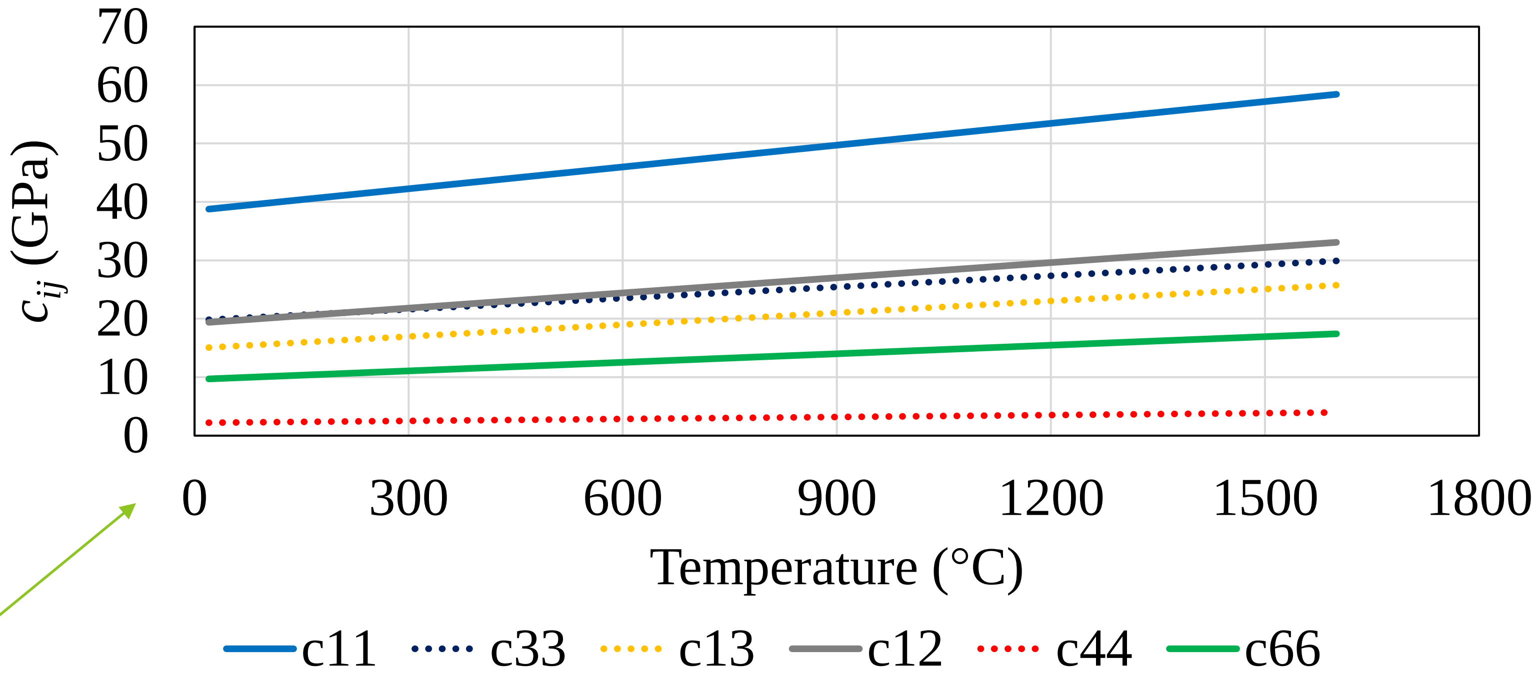
**Material's single crystal properties**
**+**
**Polycrystalline texture**

$\approx$

**Anisotropic Polycrystalline Properties**

[1] C.N. Tomé, R.A. Lebensohn, *Polycrystal thermo-elasticity revisited: theory and applications*, Cr Mecanique 348(10-11) (2020) 877-891.

# PyC $c_{ij}$ – Isotropic vs. Transversely Isotropic



Strong texture (ex. high burnup) [2] →

Isotropic →

| OA (°) | T (°C) | $c_{11}$ | $c_{22}$ | $c_{33}$ | $c_{13}$ | $c_{23}$ | $c_{12}$ | $c_{44}$ | $c_{55}$ | $c_{66}$ |
|---|---|---|---|---|---|---|---|---|---|---|
| **20** | 20 | 38.8 | 38.8 | 19.8 | 15.1 | 15.1 | 19.4 | 2.2 | 2.2 | 9.5 |
| **180** | 20 | 25.8 | 25.8 | 25.8 | 15.5 | 15.5 | 15.5 | 5 | 5 | 5 |

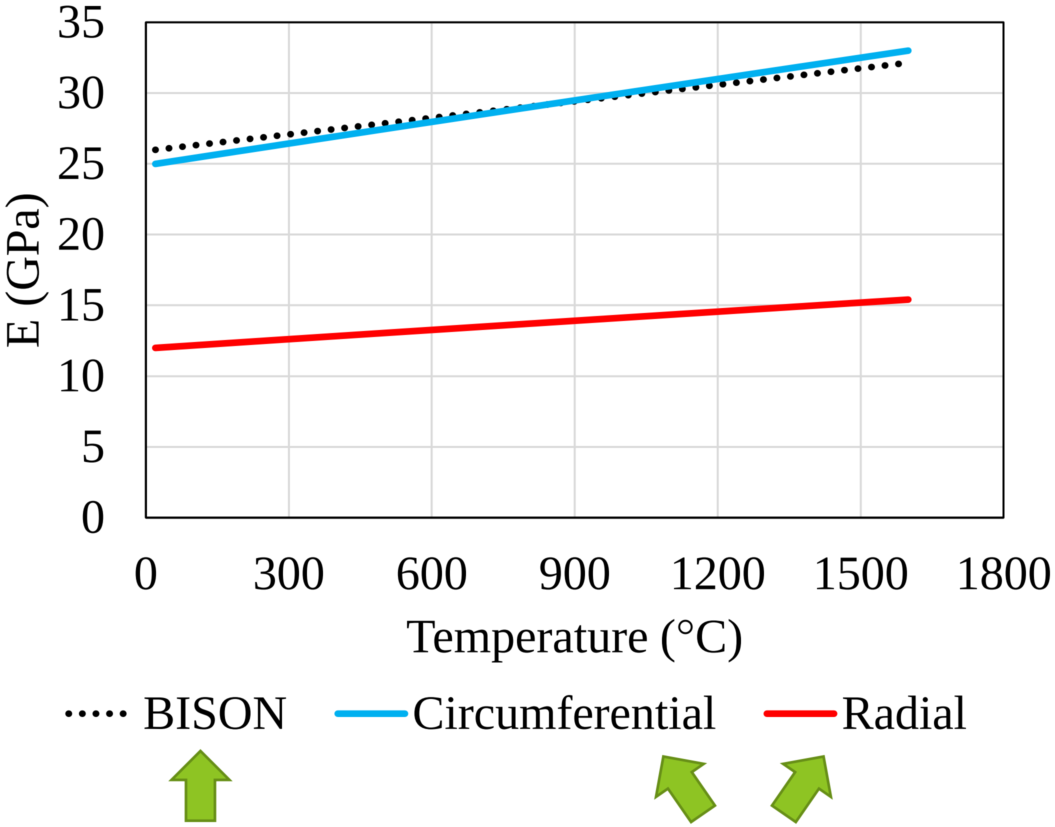
All $c_{ij}$ in GPa

[1] J.A. Evans, R.A. Lebensohn, J.R. Harter, K.D. Weaver, *Anisotropic temperature-dependent elastic constants and thermal conductivities of TRISO particle coatings*, J Nucl Mater 565 (2022).

[2] S.L. Feng, Y.G. Yang, L. Li, D.S. Zhang, X.M. Yang, S. Bai, H.H. Xia, L. Yan, P. Huai, X.T. Zhou, *Effect of Ar+ ion irradiation on the microstructure of pyrolytic carbon*, J Appl Phys 117(11) (2015).

# PyC – Engineering Constants

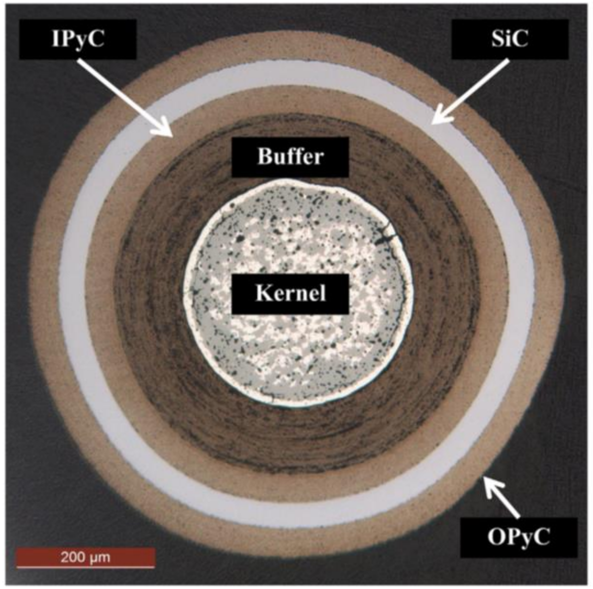
PyC Young's Moduli [1]

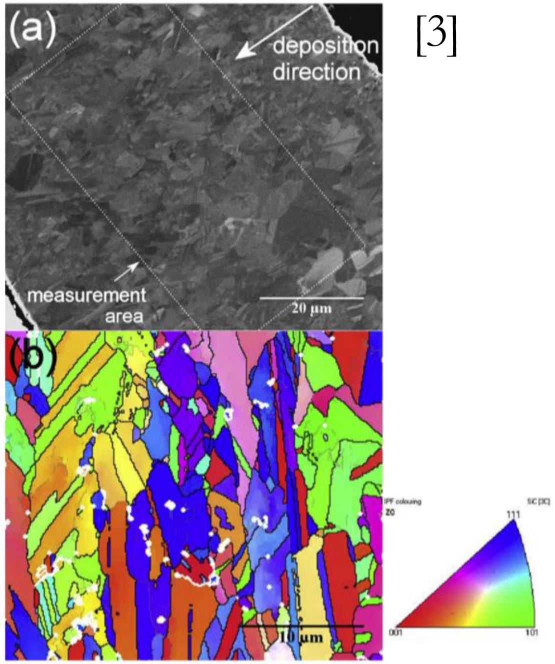


BAF = 1.1

OA = 20°

[2]





[3]

[2] R.L. Seibert, K.A. Terrani, D. Velazquez, J.D. Hunn, C.A. Baldwin, F.C. Montgomery, J. Terry, *Local atomic structure of Pd and Ag in the SiC containment layer of TRISO fuel particles fissioned to 20% burn-up*, J Nucl Mater 500 (2018) 316-326.
[3] N. Rohbeck, D. Tsivoulas, I.P. Shapiro, P. Xiao, S. Knol, J.M. Escleine, M. Perez, *In-situ nanoindentation of irradiated silicon carbide in TRISO particle fuel up to 500 degrees C*, J Nucl Mater 465 (2015) 692-694.

[1] J.A. Evans, R.A. Lebensohn, J.R. Harter, K.D. Weaver, *Anisotropic temperature-dependent elastic constants and thermal conductivities of TRISO particle coatings*, J Nucl Mater 565 (2022).

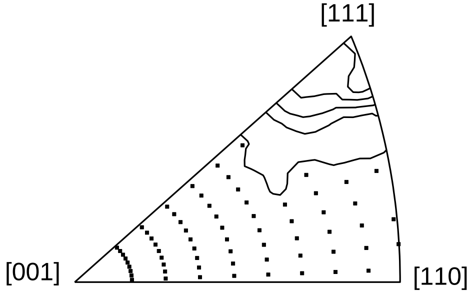
# Silicon Carbide – Elastic Constants

**(Single crystal $c_{ij}$) + (known texture) ≈⟶ Polycrystalline $c_{ij}$**

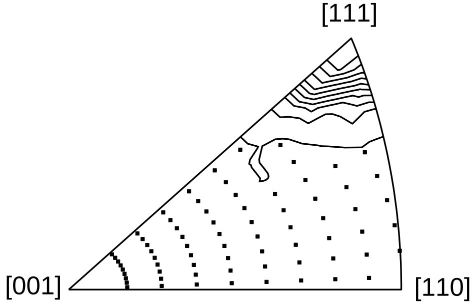
| MRD | T (°C) | $c_{11}$ | $c_{22}$ | $c_{33}$ | $c_{13}$ | $c_{23}$ | $c_{12}$ | $c_{44}$ | $c_{55}$ | $c_{66}$ |
|---|---|---|---|---|---|---|---|---|---|---|
| Single Xtal [1] | 20 | 352 | 352 | 352 | 140 | 140 | 140 | 233 | 233 | 233 |
| 10 | | 458 | 458 | 490 | 71 | 71 | 104 | 148 | 148 | 175 |
| 5 | | 456 | 456 | 483 | 75 | 75 | 102 | 151 | 151 | 174 |
| Isotropic | | 438 | 438 | 438 | 97 | 97 | 97 | 170 | 170 | 170 |
| Single Xtal [1] | 1000 | 327 | 327 | 327 | 129 | 129 | 129 | 226 | 226 | 226 |
| 10 | | 432 | 432 | 465 | 60 | 60 | 93 | 141 | 141 | 168 |
| 5 | | 430 | 430 | 457 | 64 | 64 | 91 | 143 | 143 | 166 |
| Isotropic | | 413 | 413 | 413 | 87 | 87 | 87 | 162 | 162 | 162 |

← all GPa

IPF for MRD = 5



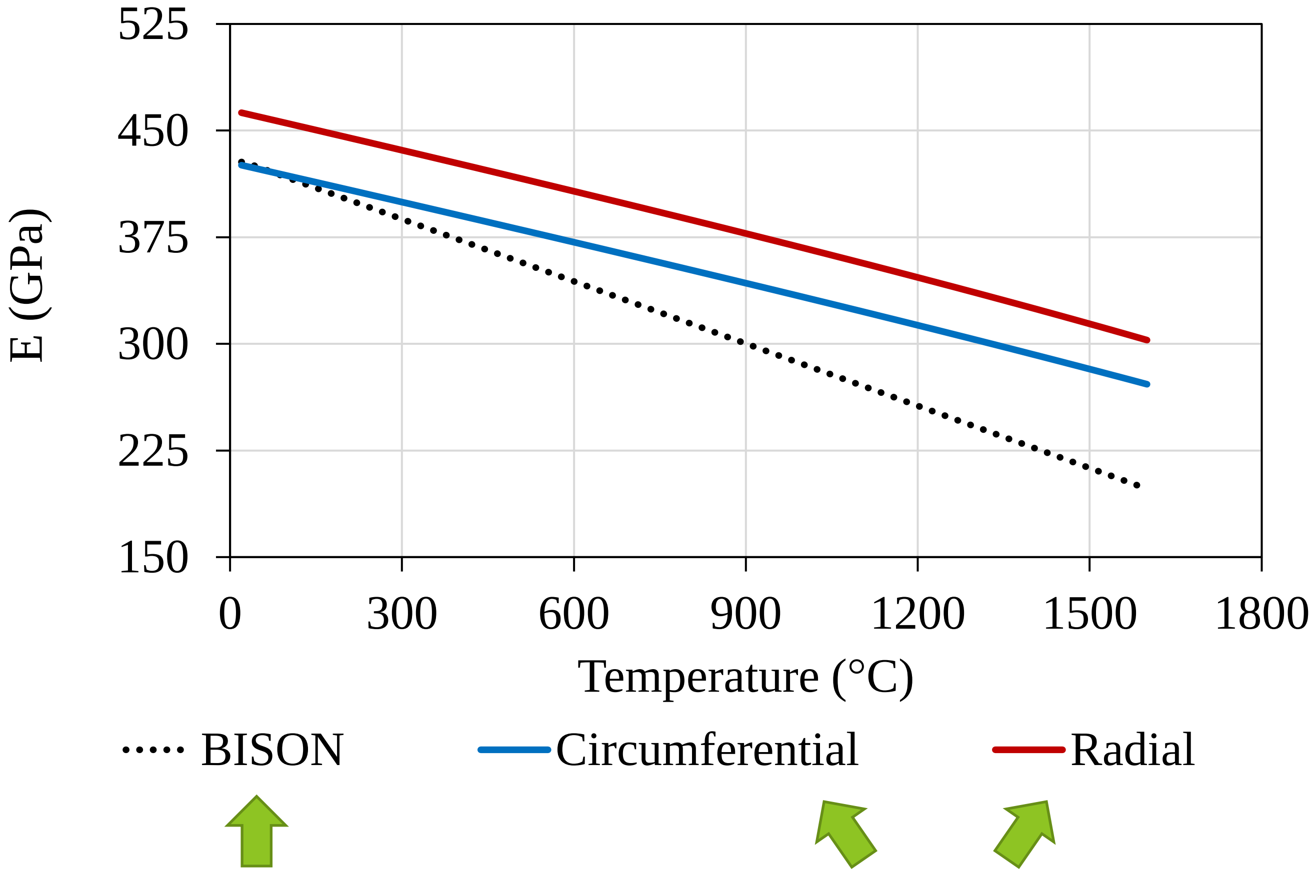
IPF for MRD = 10



[1] Z. Li, R.C. Bradt, *The single-crystal elastic-constants of cubic (3C) SiC to 1000-degrees-C*, J. Mater. Sci., 22 (7) (1987), pp. 2557-2559

[2] J.A. Evans, R.A. Lebensohn, J.R. Harter, K.D. Weaver, *Anisotropic temperature-dependent elastic constants and thermal conductivities of TRISO particle coatings*, J Nucl Mater 565 (2022).

# Silicon Carbide – Young’s Moduli



Assumes Isotropy

MRD = 5 [2]

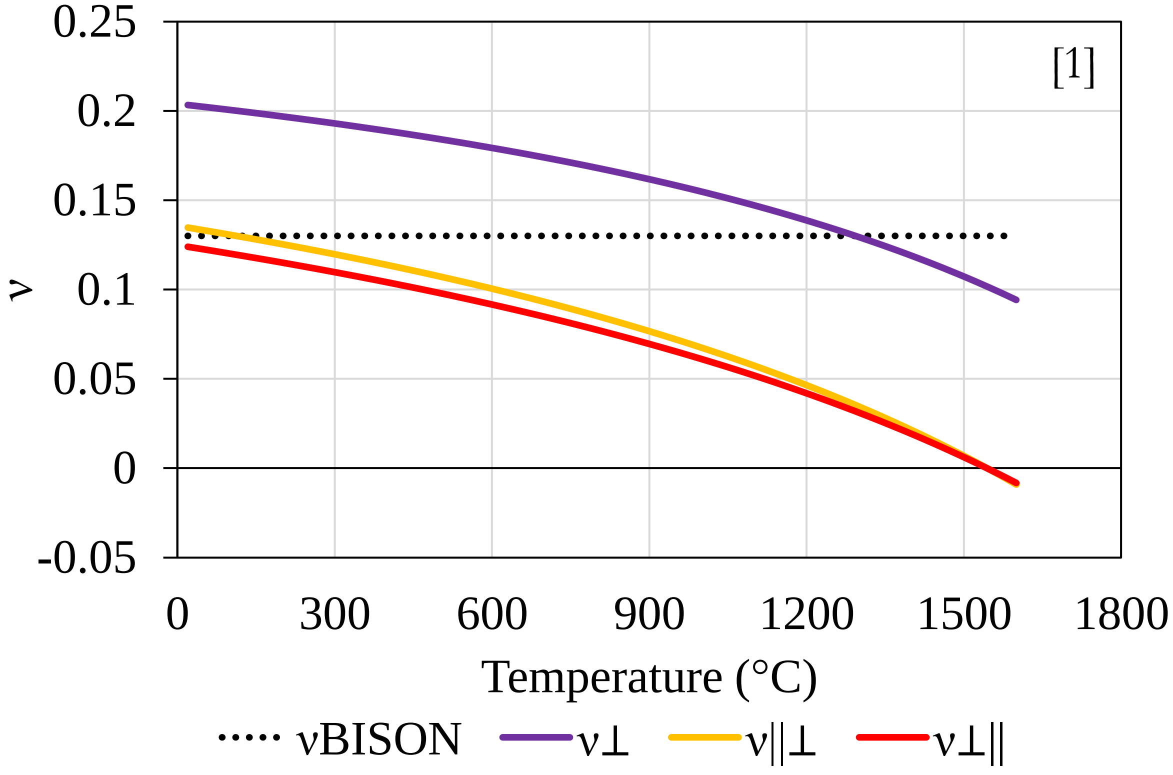
- If we assume modest SiC texture (MRD = 5, per EBSD of unirradiated TRISO)… [2]
- At RT, BISON predicts the same *E* as anisotropic circumferential *E* with MRD = 5
- Difference in slope between calculated and historical relationships
  - Cause has not been identified

[2] D. Helary, O. Dugne, X. Bourrat, P.H. Jouneau, F. Cellier, *EBSD investigation of SiC for HTR fuel particles*, J Nucl Mater 350(3) (2006) 332-335.

[1] J.A. Evans, R.A. Lebensohn, J.R. Harter, K.D. Weaver, *Anisotropic temperature-dependent elastic constants and thermal conductivities of TRISO particle coatings*, J Nucl Mater 565 (2022).

# Silicon Carbide – Poisson’s Ratios

- If we assume modest SiC texture (MRD = 5, per EBSD of unirradiated TRISO)…
- At RT, BISON predicts the same $\nu$ as anisotropic $\nu_{||\perp}$ and $\nu_{||\perp}$ with MRD = 5
- Anisotropic SiC coating becomes *auxetic* (!) at high temperatures
- Auxetic behavior has been observed in other materials, including SiC polymorphs [2,3]



Assumes Isotropy & Constant

MRD = 5

where $$\nu_{ki} = \frac{\varepsilon_{kk}}{\varepsilon_{ii}}$$

[1] J.A. Evans, R.A. Lebensohn, J.R. Harter, K.D. Weaver, *Anisotropic temperature-dependent elastic constants and thermal conductivities of TRISO particle coatings*, J Nucl Mater 565 (2022).

[2] X.B. Liu, X.F. Shao, B. Yang, M.W. Zhao, *Negative Poisson’s ratio and high-mobility transport anisotropy in SiC6 siligraphene*, Nanoscale, 10 (4) (2018), pp. 2108-2114

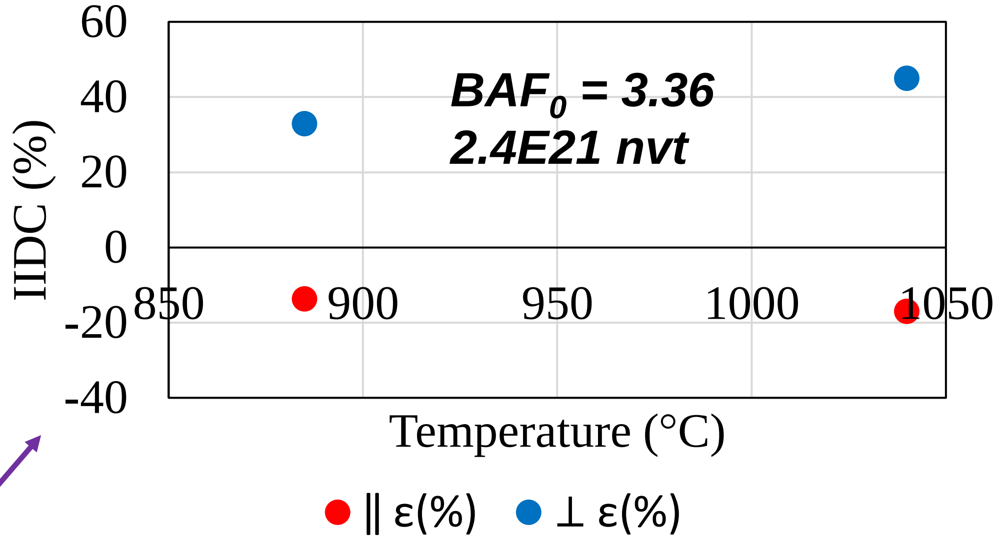
[3] R.V. Goldstein, V.A. Gorodtsov, D.S. Lisovenko, *The elastic properties of hexagonal auxetics under pressure*, Phys. Status Solidi B, 253 (7) (2016), pp. 1261-1269

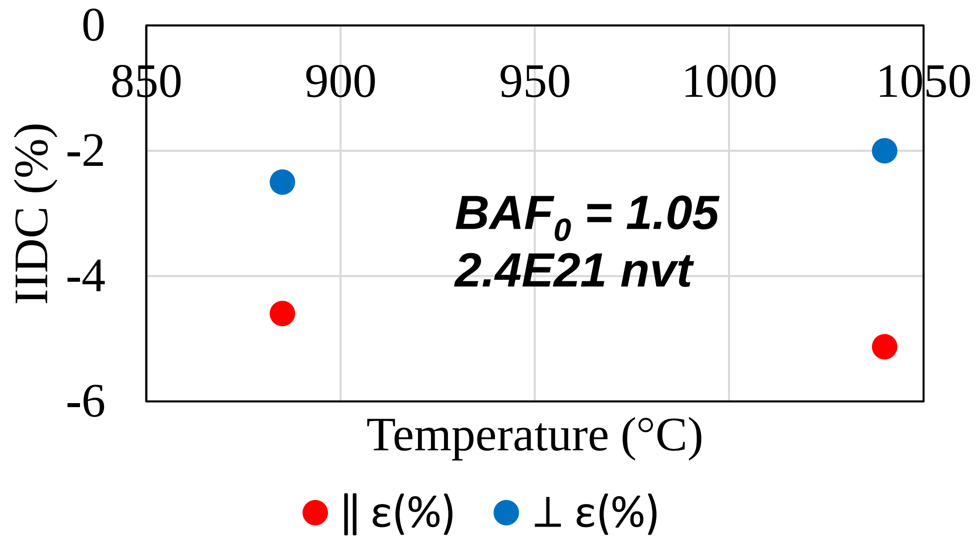
# ANISOTROPY AND TRISO FUEL PERFORMANCE

## Elastic Properties vs. Radiation Response

# Anisotropy and Fuel Performance

- The current tensorial description addresses present elastic properties *only*
- It *does not* predict radiation response/evolution
- A better description of how (a) textures evolve during irradiation and (b) how radiation response is influenced by those textures is needed
- For example, irradiation-induced dimensional changes (IIDC) in PyC are known to be strongly anisotropic when the material is strongly textured [1]





[1] J.C. Bokros, R.J. Price, *Radiation-Induced Dimensional Changes in Pyrolytic Carbons Deposited in a Fluidized Bed*, Carbon 4(3) (1966) 441-454.

# Conclusions

- TRISO particle coatings have transversely isotropic texture
- (Single Xtal $c_{ij}$) + (Texture) → (Anisotropy)
- The $c_{ij}$ (T) of TRISO coatings have been determined for selected textures
- $c_{ij}$ have been used to determine the engineering constants
  - Anisotropic SiC exhibits auxetic behavior at high temperatures
- This description *does not* relate to radiation effects
- Tensorial description of TRISO coatings has recently been implemented into BISON at INL, *however…*
- Texture vs. dose and radiation response vs. texture/anisotropy relationships are required for a fully descriptive fuel performance model (remaining work)

Funding: Contract No. DE-AC07-05ID14517 with the U.S. Department of Energy

Idaho National Laboratory

# Generalized Hooke's Law

$$\boxed{\sigma_{ij} = c_{ijkl}\varepsilon_{kl}}$$

**Isotropic**: 2 independent $c_{ij}$

$$\begin{bmatrix} \sigma_{11} \\ \sigma_{22} \\ \sigma_{33} \\ \sigma_{23} \\ \sigma_{13} \\ \sigma_{12} \end{bmatrix} = \begin{bmatrix} c_{11} & c_{12} & c_{12} & 0 & 0 & 0 \\ & c_{11} & c_{12} & 0 & 0 & 0 \\ & & c_{11} & 0 & 0 & 0 \\ & & & c_{44} & 0 & 0 \\ & sym & & & c_{44} & 0 \\ & & & & & c_{44} \end{bmatrix} \begin{bmatrix} \varepsilon_{11} \\ \varepsilon_{22} \\ \varepsilon_{33} \\ 2\varepsilon_{23} \\ 2\varepsilon_{13} \\ 2\varepsilon_{12} \end{bmatrix}$$

where $c_{12} = c_{11} - 2c_{44}$

$$E_{iso} = \frac{c_{11}^2 + c_{11}c_{12} - 2c_{12}^2}{c_{11} + c_{12}}$$

$$G_{iso} = c_{44} \qquad \nu_{iso} = \frac{c_{12}}{c_{11} + c_{12}}$$

**Transversely Isotropic**: 5 independent $c_{ij}$

$$\begin{bmatrix} \sigma_{11} \\ \sigma_{22} \\ \sigma_{33} \\ \sigma_{23} \\ \sigma_{13} \\ \sigma_{12} \end{bmatrix} = \begin{bmatrix} c_{11} & c_{12} & c_{13} & 0 & 0 & 0 \\ & c_{11} & c_{13} & 0 & 0 & 0 \\ & & c_{33} & 0 & 0 & 0 \\ & & & c_{44} & 0 & 0 \\ & sym & & & c_{44} & 0 \\ & & & & & c_{66} \end{bmatrix} \begin{bmatrix} \varepsilon_{11} \\ \varepsilon_{22} \\ \varepsilon_{33} \\ 2\varepsilon_{23} \\ 2\varepsilon_{13} \\ 2\varepsilon_{12} \end{bmatrix}$$

where $c_{12} = c_{11} - 2c_{66}$

$$E_{\parallel} = E_{rad} = \frac{c_{11}c_{33} + c_{12}c_{33} - 2c_{13}^2}{c_{11} + c_{12}}$$

$$E_{\perp} = E_{circ} = \frac{c_{11}^2 c_{33} + 2c_{13}^2 c_{12} - 2c_{13}^2 c_{11} - c_{12}^2 c_{33}}{c_{11}c_{33} - c_{13}^2}$$

[1] J.A. Evans, B.T. Sturtevant, B. Clausen, S.C. Vogel, F.F. Balakirev, J.B. Betts, L. Capolungo, R.A. Lebensohn, B. Maiorov, *Determining elastic anisotropy of textured polycrystals using resonant ultrasound spectroscopy*, J Mater Sci 56(16) (2021) 10053-10073.

# Bacon Anisotropy Factor (BAF)

- BAF is defined by the relative number of atoms in {0002} planes per unit solid angle that make an angle $\phi$ with the deposition plane normal [1]
  - $I(\phi)$ obtained from variations in intensity of the {0002} Debye-Scherrer diffraction ring
- BAF varies from unity (isotropic) to infinity (single crystal)
- BAF is often used in computational modeling of TRISO (BISON, PARFUME, etc.), ex. for PyC… [2]

$$BAF = 2 \cdot \frac{\int_0^{\pi/2} I(\phi) \cdot \cos^2\phi \cdot \sin\phi \, d\phi}{\int_0^{\pi/2} I(\phi) \cdot \sin^3\phi \, d\phi}$$

$$E = \frac{E_r + 2E_t}{3}$$

$$E_r = 25.5\left(0.384 + \rho \cdot 0.324 \times 10^{-3}\right)\overbrace{\left(1.463 - 0.463 \cdot BAF\right)}^{\textbf{Can be negative! (Not intended for strong textures)}}$$
$$\left(2.985 - 0.0662 \cdot L_c\right)\left(1 + 0.23 \cdot \phi\right)\left[1 + 0.00015\left(T - 20\right)\right]$$

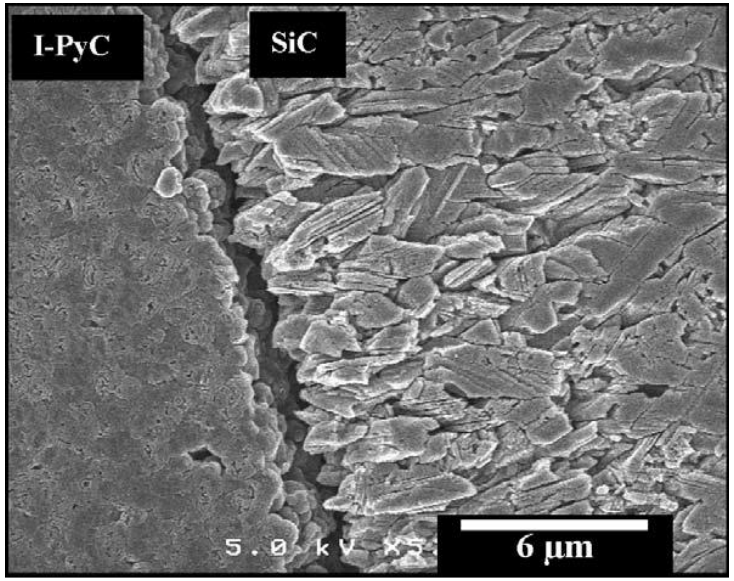
$$E_t = 25.5\left(0.384 + \rho \cdot 0.324 \times 10^{-3}\right)\left(0.481 + 0.519 \cdot BAF\right)$$
$$\left(2.985 - 0.0662 \cdot L_c\right)\left(1 + 0.23 \cdot \phi\right)\left[1 + 0.00015\left(T - 20\right)\right]$$

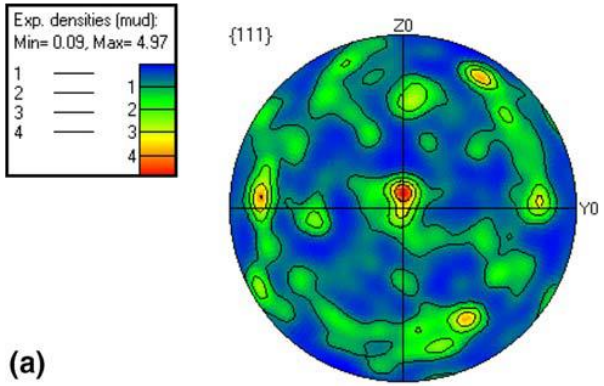
[1] G.E. Bacon, *A Method for determining the degree of orientation of graphite*, J. Appl. Chem., 6 (11) (1956), pp. 477-481

[2] J.D. Hales, R.L. Williamson, S.R. Novascone, D.M. Perez, B.W. Spencer, G. Pastore, *Multidimensional multiphysics simulation of TRISO particle fuel*, J Nucl Mater 443(1-3) (2013) 531-543.

# Multiples of Random Distribution (MRD)

- EBSD can be used to determine quantitatively measure (and map) texture
- Follows Bragg’s law of diffraction
- Texture visualized in pole figures (PFs) or inverse pole figures (IPFs)
- MRD > 1 representative of more abundant crystalline orientations
- Unirradiated SiC layer of TRISO particles can have (small, MRD ~5) transversely isotropic texture [1]
  - <111> parallel to growth (radial) direction

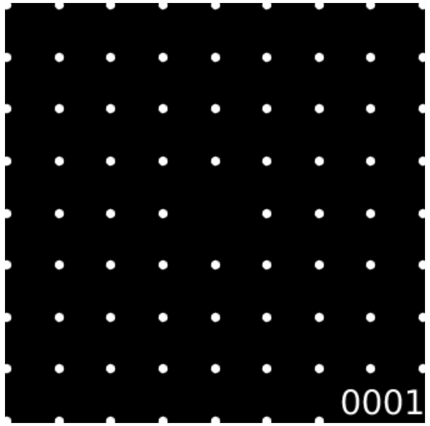


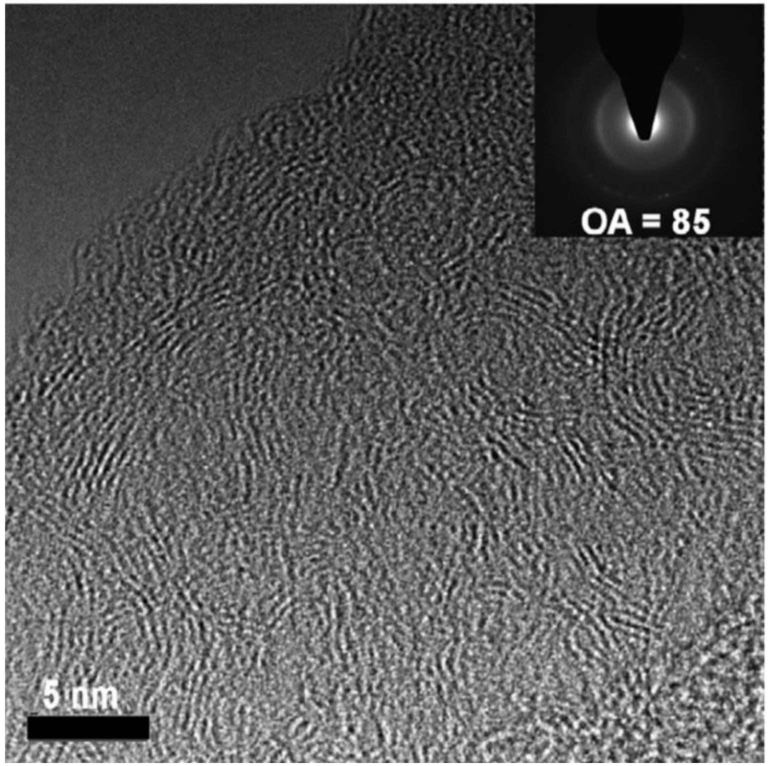


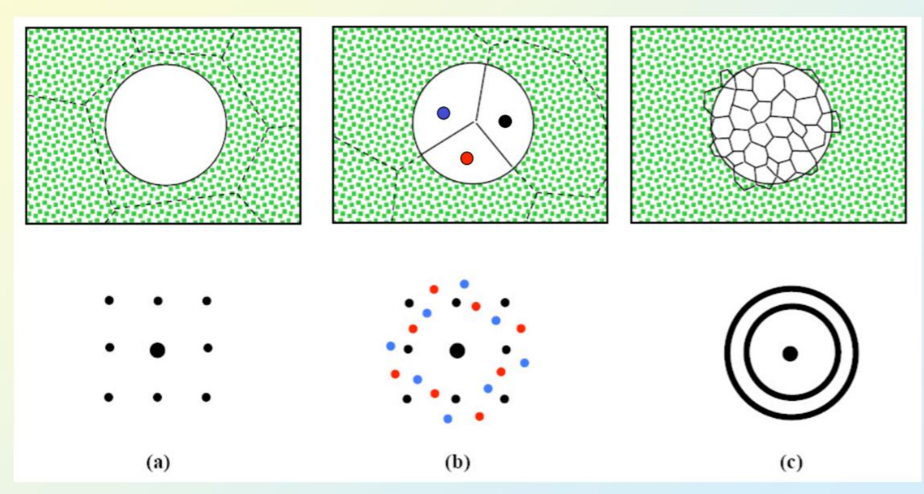
[1] D. Helary, O. Dugne, X. Bourrat, P.H. Jouneau, F. Cellier, *EBSD investigation of SiC for HTR fuel particles*, J Nucl Mater 350(3) (2006) 332-335.

# TEM Diffraction Patterns – Preamble to Orientation Angle (OA)

- TEM diffraction patterns (DPs) also follow Bragg’s law
- Crystallographic structure can be qualitatively inferred by inspection (single crystal, “multicrystal”, polycrystal)
- Untextured = rings in DPs
- Textured = rings with arc-shaped brightness variation in DPs [1]



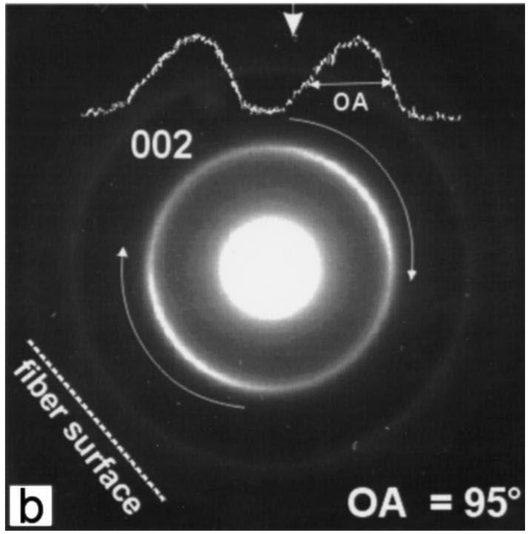


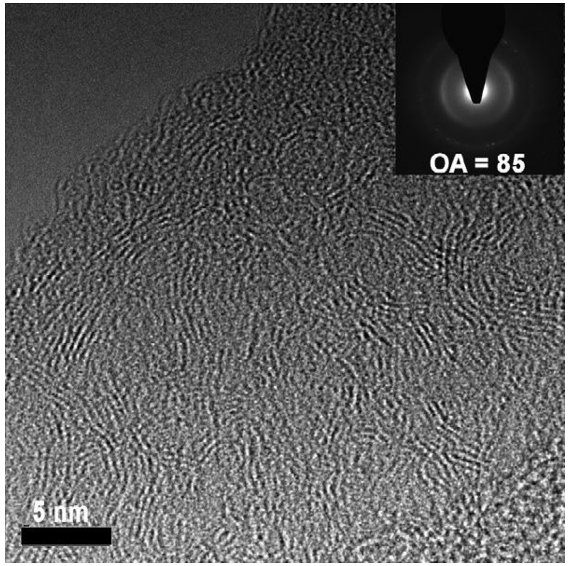


[1] E. Lopez-Honorato, P.J. Meadows, P. Xiao, G. Marsh, T.J. Abram, *Structure and mechanical properties of pyrolytic carbon produced by fluidized bed chemical vapor deposition*, Nucl Eng Des 238(11) (2008) 3121-3128.

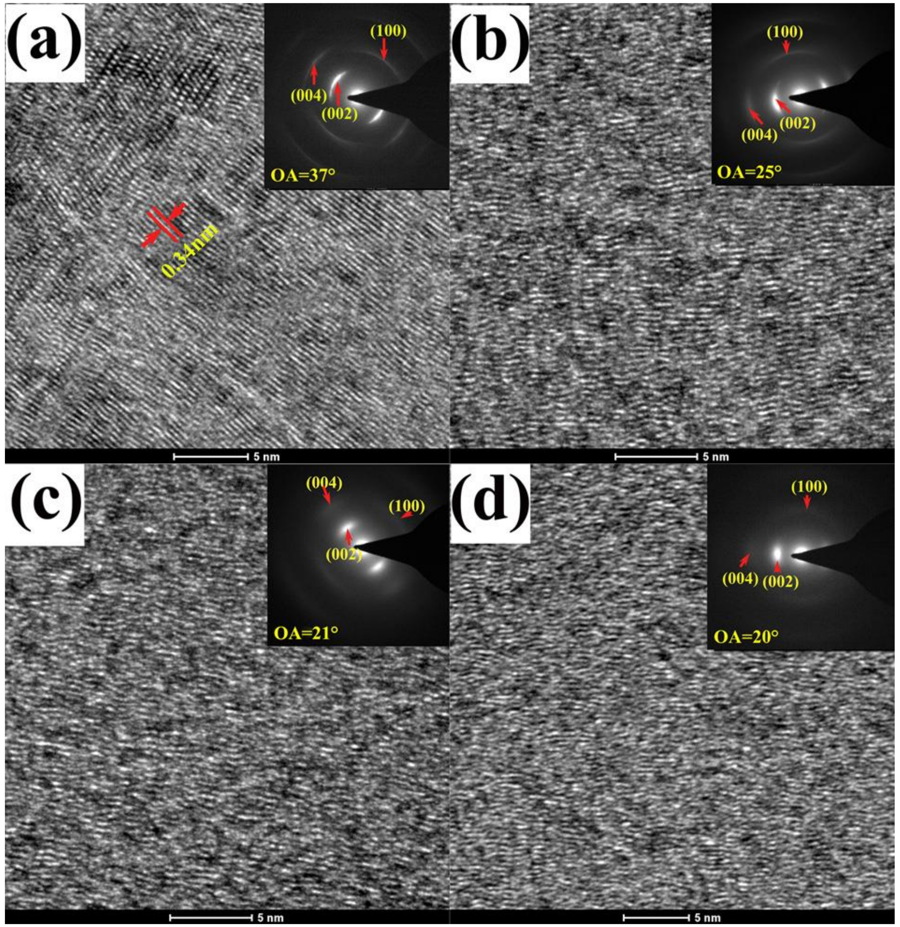
# Orientation Angle (OA)

- OA corresponds to the FWHM of the intensity maxima along the (002) reflections [1]
- OA varies from 0° (single crystal) to 180° (isotropic)
- In terms of OA (which is *non-linear*)
  - <u>Low Texture</u>: 180 > OA > 80
  - <u>Moderate Texture</u>: 80 > OA > 50
  - <u>Strong Texture</u>: OA < 50
- OA of PyC layers of 80-100° observed in as-fab TRISO [2]





OA of PyC observed to increase with radiation damage (**20° at dose of 1 dpa**) [3]



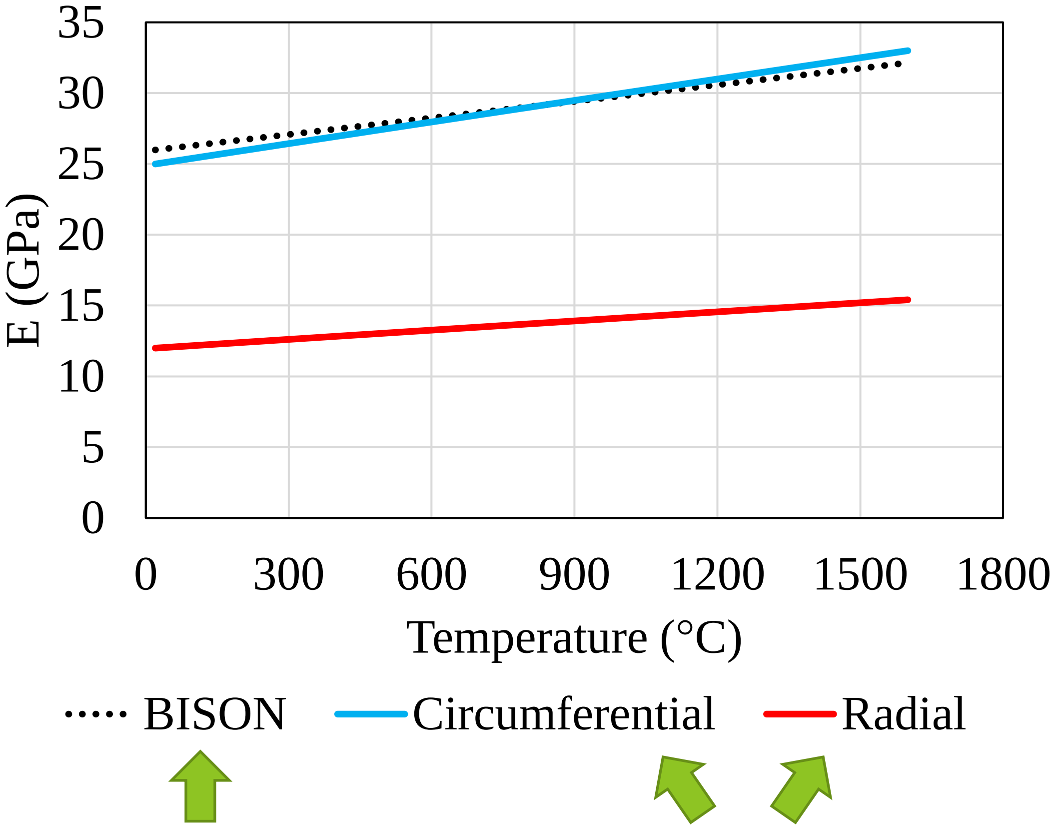
[1] B. Reznik, K.J. Huttinger, On the terminology for pyrolytic carbon, Carbon 40(4) (2002) 621-624.

[2] E. Lopez-Honorato, P.J. Meadows, P. Xiao, G. Marsh, T.J. Abram, *Structure and mechanical properties of pyrolytic carbon produced by fluidized bed chemical vapor deposition*, Nucl Eng Des 238(11) (2008) 3121-3128.

[3] S.L. Feng, Y.G. Yang, L. Li, D.S. Zhang, X.M. Yang, S. Bai, H.H. Xia, L. Yan, P. Huai, X.T. Zhou, *Effect of Ar+ ion irradiation on the microstructure of pyrolytic carbon*, J Appl Phys 117(11) (2015).

# PyC – Engineering Constants

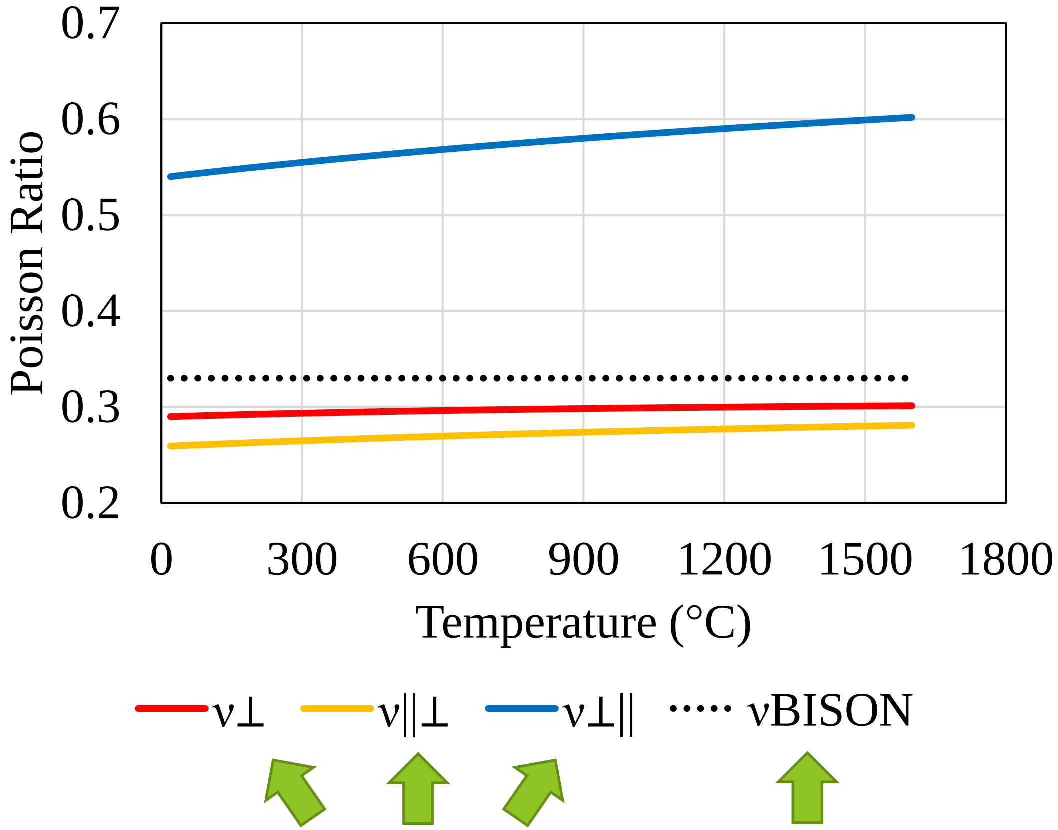
## PyC Young’s Moduli



BAF = 1.1

OA = 20°

## PyC Poisson’s Ratios



OA = 20°

BAF = 1.1

[1] J.A. Evans, R.A. Lebensohn, J.R. Harter, K.D. Weaver, *Anisotropic temperature-dependent elastic constants and thermal conductivities of TRISO particle coatings*, J Nucl Mater 565 (2022).